Unconventional critical behavior of fermions hybridized with bosons

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A phase transition into the condensed state of fermions hybridized with immobile bosons is examined beyond the ordinary mean-field approximation (MFA) in two and three dimensions. The hybridization interaction does not provide the Cooper pairing of fermions and the Bose-condensation in two-dimensions. In the three-dimensional (3D) boson-fermion model (BFM) an expansion in the strength of the order parameter near the transition yields no linear homogeneous term in the Ginzburg-Landau-Gor'kov equation. This indicates that previous mean-field discussions of the model are flawed in any dimensions. In particular, the conventional (MFA) upper critical field is zero in any-dimensional BFM

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Soon after Anderson [1] and Street and Mott [2] introduced localized electron pairs to explain some unusual properties of chalcogenide glasses, a two component model of negative U centers coupled with the Fermi sea of itinerant fermions was employed to study superconductivity in disordered metal-semiconductor alloys [3, 4]. When the attractive potential U is large, the model is reduced to localized hard-core bosons spontaneously decaying into itinerant electrons and vice versa, different from a non-converting mixture of mobile charged bosons and fermions [5, 6]. Later on the model was applied more generally to describe pairing electron processes with localization-delocalization [7], and a linear resistivity in the normal state of cuprates [8]. The model attracted more attention in connection with high-temperature superconductors [9, 10, 11, 12, 13, 14, 15]. In particular, Refs. [14, 15] claimed that 2D BFM with immobile hard-core bosons is capable to reproduce some physical properties and the phase diagram of cuprates.

The model is defined by the Hamiltonian,

$$H = \sum_{\mathbf{k},\sigma=\uparrow,\downarrow} \xi_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + E_0 \sum_{\mathbf{q}} b^{\dagger}_{\mathbf{q}} b_{\mathbf{q}} + \mathrm{g}N^{-1/2} \sum_{\mathbf{q},\mathbf{k}} \left(\phi_{\mathbf{k}} b^{\dagger}_{\mathbf{q}} c_{-\mathbf{k}+\mathbf{q}/2,\uparrow} c_{\mathbf{k}+\mathbf{q}/2,\downarrow} + H.c. \right), \tag{1}$$

where $\xi_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - \mu$ is the 2D energy spectrum of fermions, $E_0 \equiv \Delta_B - 2\mu$ is the bare boson energy with respect to the chemical potential μ, g is the magnitude of the anisotropic hybridization interaction, $\phi_{\mathbf{k}} = \phi_{-\mathbf{k}}$ is the anisotropy factor, and N is the number of cells. Ref. [14] argued that 'superconductivity is induced in this model from the anisotropic charge exchange (hybridization) interaction ($\mathrm{g}\phi_{\mathbf{k}}$) between the conduction-band fermions and the immobile hard-core bosons', and 'the on-site Coulomb repulsion competes with this pairing' reducing the critical temperature T_c less than by 25%. Also it has been argued [15], that the calculated upper critical field of the model fits well the experimental results.

This, as well as some other studies of BFM applied a mean-field approximation (MFA) to the condensed phase of BFM, replacing zero-momentum boson operators by c-numbers and neglecting the boson self-energy. MFA led to a conclusion that 'bosons exist only as virtual state' at sufficiently large boson energy E_0, so that BFM exhibits features compatible with BCS characteristics with a relatively small fluctuation region Gi[12], and describes a crossover from the BCS-like to local pair behavior [9, 10, 14]. However, our study of BFM [13] beyond MFA revealed a crucial effect of the boson self-energy on the normal state boson spectral function. The energy of zero-momentum bosons is renormalized down to *zero* at the critical temperature $T = T_c$, no matter how weak the boson-fermion coupling and how large the bare boson energy are. As a result, the Cooper pairing of fermions via *virtual unoccupied* bosonic states is impossible, but it could occur only simultaneously with the Bose-Einstein condensation of *real* bosons in BFM.

Here I show that there is no BCS-like condensed state in the two-dimensional model. More surprisingly, the mean-field approximation appears meaningless even in three-dimensional BFM because of the complete boson softening. The phase transition is never a BCS-like second-order phase transition. In particular, the conventional upper critical field is zero in 3D BFM.

Replacing boson operators by c-numbers for $\mathbf{q} = 0$ in Eq.(1) one obtains a linearised BCS-like equation for the fermion order-parameter $\Delta_{\mathbf{k}}$,

$$\Delta_{\mathbf{k}} = \frac{\tilde{\mathrm{g}}^2 \phi_{\mathbf{k}}}{E_0 N} \sum_{\mathbf{k}'} \phi_{\mathbf{k}'} \frac{\Delta_{\mathbf{k}'} \tanh(\xi_{\mathbf{k}'}/2k_B T)}{2\xi_{\mathbf{k}'}}, \tag{2}$$

with the coupling constant $\tilde{\mathrm{g}}^2 = \mathrm{g}^2(1 - 2n^B)$, renormalized by the hard-core effects. Using a two-particle fermion vertex part in the Cooper channel one can prove that this equation is perfectly correct even beyond the conventional non-crossing approximation [13]. Nevertheless, the problem with MFA stems from an incorrect definition of the bare boson energy with respect to the chemical potential, $E_0(T)$. This energy is determined by the atomic density of bosons (n^B) as (Eq.(9) in Ref. [14])

$$\tanh \frac{E_0}{2k_B T} = 1 - 2n^B. \tag{3}$$

While Eq.(2) is correct, Eq.(3) is incorrect because the

boson self-energy $\Sigma_b(\mathbf{q},\Omega_n)$ due to the same hybridization interaction is missing. At first sight [14] the self-energy is small in comparison to the kinetic energy of fermions, if g is small. However $\Sigma_b(0,0)$ diverges logarithmically at zero temperature [13], no matter how week the interaction is. Therefore it should be kept in the density sum-rule, Eq.(3). Introducing the boson Green's function

$$D(\mathbf{q},\Omega_n)=\frac{1-2n^B}{i\Omega_n-E_0-\Sigma_b(\mathbf{q},\Omega_n)} \tag{4}$$

one must replace incorrect Eq.(3) by

$$-\frac{k_BT}{N}\sum_{\mathbf{q},n}e^{i\Omega_n\tau}D(\mathbf{q},\Omega_n)=n^B, \tag{5}$$

where $\tau=+0$, and $\Omega_n=2\pi k_BTn$ $(n=0,\pm1,\pm2...)$. The divergent (cooperon) contribution to $\Sigma_b(\mathbf{q},\Omega_n)$ is given by [13]

$$\Sigma_b(\mathbf{q},\Omega_n)=-\frac{\tilde{\mathrm{g}}^2}{2N}\sum_{\mathbf{k}}\phi^2_{\mathbf{k}}\times \tag{6}$$
$$\frac{\tanh[\xi_{\mathbf{k-q/2}}/(2k_BT)]+\tanh[\xi_{\mathbf{k+q/2}}/(2k_BT)]}{\xi_{\mathbf{k-q/2}}+\xi_{\mathbf{k+q/2}}-i\Omega_n},$$

so that one obtains

$$\Sigma_b(\mathbf{q},0)=\Sigma_b(0,0)+\frac{q^2}{2M^*}+\mathcal{O}(q^4) \tag{7}$$

for small $\mathbf{q}$ with any anisotropy factor compatible with the point-group symmetry of the cuprates. Here M^* is the boson mass, calculated analytically in Ref.[13] with the isotropic exchange interaction and parabolic fermion band dispersion (see also Ref.[16]), and $\hbar=1$. The BCS-like equation (2) has a nontrivial solution for $\Delta_{\mathbf{k}}$ at $T=T_c$, if

$$E_0=-\Sigma_b(0,0). \tag{8}$$

Substituting Eq.(7) and Eq.(8) into the sum-rule, Eq.(5) one obtains a logarithmically divergent integral with respect to $\mathbf{q}$, and

$$T_c=\frac{const}{\int_0 dq/q}=0. \tag{9}$$

The devastating result, Eq.(9) is a direct consequence of the well-known theorem, which states that BEC is impossible in 2D. This is true for non-interacting bosons. Remarkably it appears also true for bosons hybridized with fermions in 2D, Eq.(9). Any dynamic repulsion between bosons could provide an infrared cut-off of the integral in Eq.(9) resulting in a finite critical temperature in 2D. But it has to be treated beyond MFA level [17, 18], and in no way does it make MFA [14, 15] a meaningful approximation.

One may erroneously believe that MFA results can be still applied in three-dimensions. However, increasing dimensionality does not make MFA a meaningful approximation either. This approximation leads to a naive conclusion that a BCS-like superconducting state occurs below the critical temperature $T_c\simeq\mu\exp(-E_0/z_c)$ via fermion pairs being *virtually* excited into *unoccupied virtual* bosonic states [9, 10, 12]. Here $z_c=\tilde{g}^2N(0)$ and $N(0)$ is the density of states (DOS) in the fermionic band near the Fermi level μ. However, the Cooper pairing of fermions is not possible via virtual unoccupied bosonic states in 3D BFM either. Indeed, Eq.(8) does not depend on the dimensionality, so that the analytical continuation of Eq.(4) to real frequencies ω yields the partial boson DOS as $\rho(\omega)=(1-2n_B)\delta(\omega)$ at $T=T_c$ for $\mathbf{q}=0$ in any-dimensional BFM and for any coupling with fermions. Hence, the Cooper pairing may occur only simultaneously with the Bose-Einstein condensation of real bosons in 3D BFM [13]. The origin of the simultaneous condensation of the fermionic and bosonic fields in 3D BFM lies in the complete softening of the boson mode at $T=T_c$ caused by its hybridization with fermions.

Taking into account the boson damping and dispersion shows that the boson spectrum significantly changes for all momenta. Continuing the self-energy, Eq.(6) to real frequencies yields the damping (i.e. the imaginary part of the self-energy) as [13]

$$\gamma(\mathbf{q},\omega)=\frac{\pi z_c}{4q\xi}\ln\left[\frac{\cosh(q\xi+\omega/(4k_BT_c))}{\cosh(-q\xi+\omega/(4k_BT_c))}\right], \tag{10}$$

where $\xi=v_F/(4k_BT_c)$ is a coherence length. The damping is significant when $q\xi<<1$. In this region $\gamma(\mathbf{q},\omega)=\omega\pi z_c/(8k_BT_c)$ is comparable or even larger than the boson energy ω. Hence bosons look like overdamped diffusive modes, rather than quasiparticles in the long-wave limit [13, 16], contrary to the erroneous conclusion of Ref.[11], that there is 'the onset of coherent free-particle-like motion of the bosons' in this limit. Only outside the long-wave region, the damping becomes small. Indeed, using Eq.(10) one obtains $\gamma(\mathbf{q},\omega)=\omega\pi z_c/(2qv_F)<<\omega$, so that bosons at $q>>1/\xi$ are well defined quasiparticles with a logarithmic dispersion, $\omega(q)=z_c\ln(q\xi)$ [13]. As a result the bosons disperse over the whole energy interval from zero up to E_0.

The main mathematical problem with MFA stems from the density sum rule, Eq.(5) which determines the chemical potential of the system and consequently the bare boson energy $E_0(T)$ as a function of temperature. In the framework of MFA one takes the bare boson energy in Eq.(2) as a temperature independent parameter, $E_0=z_c\ln(\mu/T_c)$ [12], or determines it from the conservation of the total number of particles, Eq.(3) neglecting the boson self-energy $\Sigma_b(\mathbf{q},\Omega)$ [9, 10, 14, 15]). Then Eq.(2) looks like a conventional Ginzburg-Landau-Gor'kov equation [19] linearized near the transition with a negative coefficient $\alpha\propto T-T_c<0$ at $T<T_c$,

$$\alpha\Delta(\mathbf{r})=0, \tag{11}$$

where

$$\alpha = 1 + \frac{\Sigma_b(0,0)}{E_0} \approx 1 - \frac{g^2 N(0)}{E_0} \ln \frac{\mu}{T}. \qquad (12)$$

Hence, one concludes that the phase transition is almost a conventional BCS-like transition, at least at $E_0 \gg T_c$ [9, 10, 12]. Also, using the Gor'kov expansion in powers of Δ in the external field, one finds a finite upper critical field $H_{c2}(T)$ [15].

However, these findings are mathematically and physically flawed. Indeed, the term of the sum in Eq.(5) with $\Omega_n = 0$ is given by the integral

$$T \int \frac{d\mathbf{q}}{2\pi^3} \frac{1}{E_0 + \Sigma_b(\mathbf{q}, 0)}. \qquad (13)$$

The integral converges, if and only if $E_0 \geqslant -\Sigma_b(0,0)$. Hence the coefficient $\alpha(T)$ in Eq.(11) can not be negative at any temperature below T_c contrary to the MFA result [12, 15], which violates the density sum-rule predicting a wrong negative $\alpha(T)$.

Since $\alpha(T) \geqslant 0$, the phase transition is never a BCS-like second-order phase transition even at large E_0 and small g. In fact, the transition is driven by the Bose-Einstein condensation of *real* bosons with $\mathbf{q} = 0$, which occur due to the complete softening of their spectrum at T_c in 3D BFM. Remarkably, the conventional upper critical field, determined as the field, where a non-trivial solution of the linearised Gor'kov equation [19] in the external field occurs, is zero in 3D BFM, $H_{c2}(T) = 0$, because $\alpha(T) \geqslant 0$ below T_c (for more details see [21]). It is not a finite $H_{c2}(T)$ found in Ref. [15] using MFA. Of course, like in 2D BFM, the dynamic repulsion between bosons could provide a finite $H_{c2}(T)$ in 3D BFM, similar to the case of intrinsically mobile 3D bosons [20]. However, to provide a finite $H_{c2}(T)$ the dynamic repulsion has to be treated beyond MFA, as discussed in Ref. [20]. Even at temperatures well below T_c the condensed state is fundamentally different from the BCS-like MFA ground state, because of the *pairing* of bosons [21]. It is similar to a pairing of supracondensate helium atoms in ^4He, proposed as an explanation for a low density of the single-particle condensate[22]. The boson pairing appears in 3D BFM due to the hybridization of bosons with fermionic condensate. It is not expected in the framework of MFA, where the effective interaction between bosons was found repulsive by integrating out the fermionic degrees of freedom with an incorrect (constant) E_0 [12]. The pair-boson condensate should significantly modify the thermodynamic properties of the condensed BFM compared with the MFA predictions.

This qualitative failure of MFA might be rather unexpected, if one believes that bosons in Eq.(1) play the same role as phonons in the BCS superconductor. This is not the case for two reasons. The first one is the density sum-rule, Eq.(5), for bosons which is not applied to phonons. The second being that the boson self-energy is given by the divergent (at $T = 0$) Cooperon diagram, while the self-energy of phonons is finite at small coupling.

I conclude that MFA results for the boson-fermion model do make any sense neither in two nor in three dimensions, because the divergent self-energy has been neglected in calculating T_c and $H_{c2}(T)$. Any repulsion between bosons, induced by hard-core effects and/or by hybridization with fermions could not make MFA results [9, 10, 11, 12, 14, 15] meaningful. It is well known that the "infrared-save" 2D theory by Popov and others [17, 18] is actually *not* a mean-field theory. In 3D BFM the phase transition is due to the Bose condensation of real bosons rather than virtual ones. Hence, the mean-field theory cannot be applied for a description of 3D BFM either. There is no BCS-like state in any-dimensional BFM, and no BCS to local pair crossover. The common wisdom that at weak coupling the boson-fermion model is adequately described by the BCS theory, is negated by our results.

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